arXiv:cond-mat/0402674v1 [cond-mat.mes-hall] 27 Feb 2004

Spin swap vs. double occupancy in quantum gates

T. A. Kaplan and C. Piermarocchi
Department of Physics and Astronomy and Institute for Quantum Sciences, Michigan State University, East Lansing, Michigan 48824
(Dated: February 2, 2008)

We propose an approach to realize quantum gates with electron spins localized in a semiconductor that uses double occupancy to advantage. With a fast (non-adiabatic) time control of the tunnelling, the probability of double occupancy is first increased and then brought back exactly to zero. The quantum phase built in this process can be exploited to realize fast quantum operations. We illustrate the idea focusing on the half-swap operation, which is the key two-qubit operation needed to build a CNOT gate.

PACS numbers: 75.10.Pq

Many solid state proposals for quantum computation make use of the spin of an electron localized in a quantum dot [1, 2] or by a donor ion [3] as a qubit. In these schemes the overlap between the electron wave functions in neighboring dots is controlled by gates, and the exchange interaction provides the mechanism for the realization of conditional operations on two qubits. Among the requirements for such proposals is that one wants no or small double occupancy, i.e. small probability to have the two electrons in the same dot or donor. In fact, the state space $\mathcal{S}$ for 2 qubits has to be 4-dimensional and the mixing with the states of double occupancy brings the physical system out of the computational space. Hu and Das Sarma [4] observed that the double occupancy will in principle degrade any implementation of quantum gates, and noted the intrinsic conflict of trying to minimize this double occupancy while making the overlap large enough to realize a sizeable two-qubit operation, like e.g. a spin swap. The problem was further analyzed in Ref. [5], where it was shown that using an adiabatic control in the quantum dots case, the double occupancy was small enough so that the degradation can be made negligible, consistently with the requirement of large enough overlap. The operation critical to quantum computing is the *half-swap* operation (also written as $\sqrt{SWAP}$), i.e. having the state going half of the way to the complete swap, and we focus on this process to illustrate the approach.

We show here that *a half-swap operation without degradation can be realized by designing a time control where the probability of double occupancy first increases and then is brought back exactly to zero. In this cycle the quantum state in $\mathcal{S}$ picks up a phase that is exploited in completing the process.* As a consequence, the swap can be much faster than that in the case where double occupancy is kept small at all times. We will consider explicitly two cases where the control of the tunneling amplitude follows in time a square and a hyperbolic secant pulse shape. The conditions for a perfect $\sqrt{SWAP}$, i. e. a fast half-swap gate with double occupancy identically zero, can be given in these two cases by simple analytic rules. The results are exact within the single band model considered, the validity of which will be discussed below for realistic systems.

The dynamics during the half swap can be described by using two spatial orbitals, which we call w_a and w_b (w for Wannier functions), orthonormal, and localized respectively around the two sites a and b [4, 5, 6]. The w's are linear combinations of non-orthogonal "atomic" functions whose overlap is Λ. This implies a 4-state one-electron basis, and therefore a 6-dimensional complete vector space for 2 electrons. [7] The Hamiltonian H contains the kinetic and potential energies, plus a magnetic field interacting with the orbital magnetic moment. The quantum control is realized by changing the profile of the potential energy, therefore modifying the tunnelling amplitude between the two sites. We will not consider a magnetic field term, since it is irrelevant in the proposed scheme. The 2-electron basis used is

$$|\Phi_1\rangle = 2^{-1/2}(c^\dagger_{a\uparrow}c^\dagger_{b\downarrow} - c^\dagger_{a\downarrow}c^\dagger_{b\uparrow})|0\rangle \quad (1a)$$

$$|\Phi_2\rangle = 2^{-1/2}(c^\dagger_{a\uparrow}c^\dagger_{a\downarrow} + c^\dagger_{b\uparrow}c^\dagger_{b\downarrow})|0\rangle \quad (1b)$$

$$|\Phi_3\rangle = 2^{-1/2}(c^\dagger_{a\uparrow}c^\dagger_{a\downarrow} - c^\dagger_{b\uparrow}c^\dagger_{b\downarrow})|0\rangle \quad (1c)$$

$$|\Phi_4\rangle = c^\dagger_{a\uparrow}c^\dagger_{b\uparrow}|0\rangle \quad (1d)$$

$$|\Phi_5\rangle = 2^{-1/2}(c^\dagger_{a\uparrow}c^\dagger_{b\downarrow} + c^\dagger_{a\downarrow}c^\dagger_{b\uparrow})|0\rangle \quad (1e)$$

$$|\Phi_6\rangle = c^\dagger_{a\downarrow}c^\dagger_{b\downarrow}|0\rangle \ , \quad (1f)$$

where $c^\dagger_{\nu\sigma}$ creates an electron in the orbital w_ν with spin σ. Physically we speak of Φ_ν with $\nu = 1, 4, 5, 6$ as having 1 electron near each site, while for $\nu = 2, 3$, the states have 2 electrons on one site, and are called doubly-occupied states. Assuming inversion symmetry, the time-dependent Hamiltonian $H_{ij}(t) \equiv \langle\Phi_i|H(t)|\Phi_j\rangle$ reduces by symmetry to four 1×1's (the triplet H_{44}, H_{55}, and H_{66}, and the *ungerade* singlet H_{33}), plus a 2×2 which yields the remaining two (*gerade*) singlets. We assume that before applying the control pulse, at time $t = -\infty$, the wave function is $|\Psi(-\infty)\rangle = c^\dagger_{a\uparrow}c^\dagger_{b\downarrow}|0\rangle = 2^{-1/2}(|\Phi_1\rangle + |\Phi_5\rangle)$. Given the form of the initial state and the symmetry properties discussed above, $|\Phi_3\rangle$, $|\Phi_4\rangle$

and $|\Phi_6\rangle$ do not enter in the dynamics and we calculate $|\Psi(t)\rangle = a(t)|\Phi_1\rangle + b(t)|\Phi_2\rangle + c(t)|\Phi_5\rangle$ by the (time-dependent) Schrödinger equation

$$i\frac{d}{dt}\begin{bmatrix} a(t) \\ b(t) \\ c(t) \end{bmatrix}^T = \begin{bmatrix} 0 & \frac{\Omega(t)}{2} & 0 \\ \frac{\Omega(t)}{2} & \Delta & 0 \\ 0 & 0 & J_P(t) \end{bmatrix} \begin{bmatrix} a(t) \\ b(t) \\ c(t) \end{bmatrix} \qquad (2)$$

where $\hbar\Omega(t) = 2H_{12}(t)$, $\hbar\Delta = H_{22} - H_{11}$ and $\hbar J_P(t) = H_{55}(t) - H_{11}(t)$. Notice that $\Omega(t)$ is first order in the overlap Λ, while Δ depends only on the on-site and long-range Coulomb interaction: $\hbar\Delta = \langle w_a, w_a|v|w_a, w_a\rangle - \langle w_a, w_b|v|w_a, w_b\rangle$, where v is the Coulomb interaction between the two electrons. This term is of order Λ^0, and therefore only weakly dependent on the tunnelling amplitude. So we assume Δ constant during the gate operation. $\hbar J_P(t) = -2\langle w_a, w_b|v|w_b, w_a\rangle$ is the potential exchange [8], which is $O(\Lambda^2)$. The hopping term $\hbar\Omega(t) = 4\langle w_a|h_1|w_b\rangle + 4\langle w_a, w_b|v|w_a, w_a\rangle$, where h_1 is the single particle kinetic and potential energy, is responsible for the kinetic exchange. Both $J_P(t)$ and $\Omega(t)$ are controlled by the tunnelling amplitude through their dependence on the overlap Λ. We remark that these parameters simplify in the Hubbard model to $J_P(t) = 0$ and $\hbar\Delta = U$. In this case the hopping amplitude $\Omega(t)$ is the only mechanism for the exchange interaction ($J_K \cong -\hbar^2\Omega(t)^2/2U$ for small Λ, the kinetic exchange [8]). The presence of the potential exchange $J_P(t)$ is not essential in the realization of the proposed scheme, but we keep it in order to prove the reliability of the scheme in the most general case.

It is now simple to calculate the quantities we want to monitor. One is the expectation value of $s_z = n_{a\uparrow} - n_{a\downarrow}$, the z-component of spin at site a. (n_c are occupation numbers.) It is sufficient to consider just one site since the total z-component of spin is conserved and so must remain 0. Using the property $s_z|\Phi_1\rangle = |\Phi_5\rangle$, $s_z|\Phi_5\rangle = |\Phi_1\rangle$, and $s_z|\Phi_2\rangle = 0$, we find

$$\sigma_z(t) \equiv \langle\Psi(t)|s_z|\Psi(t)\rangle = 2Re[a(t)c^*(t)] \ . \qquad (3)$$

We also want the probability P_d of double occupancy, i.e. the probability of finding the system in the state Φ_2. This is

$$P_d(t) = |\langle\Phi_2|\Psi(t)\rangle|^2 = |b(t)|^2 \ . \qquad (4)$$

In order to have the perfect $\sqrt{SWAP}$ at the end of the pulse, i.e. at $t = +\infty$, we need to design the control in such a way that the two conditions

$$P_d(+\infty) = 0 \qquad (5a)$$
$$\sigma_z(+\infty) = 0 \qquad (5b)$$

are verified. One can see that Eq. (5) implies $|\Psi(+\infty)\rangle = 2^{-1/2}(c^\dagger_{a\uparrow}c^\dagger_{b\downarrow} \pm ic^\dagger_{a\downarrow}c^\dagger_{b\uparrow})|0\rangle$ (Bell entangled states). In the usual approach a weaker constraint than the one in Eq. (5a) is used (i.e. $P_d(+\infty) \ll 1$) satisfied by slow adiabatic switching and small mixing with doubly occupied states. This condition is implicit when we describe the system of two localized electrons using the (effective) Heisenberg Hamiltonian. Our approach consists in finding first the general conditions on the control to satisfy exactly Eq. (5a), which does not imply necessarily adiabaticity and small average mixing with the doubly occupied states, and then adjust the remaining control parameters to satisfy Eq. (5b).

The time dependence of $c(t)$ can be integrated directly from the Schroedinger equation and we obtain

$$c(+\infty) = 2^{-1/2}\exp(-i\int_{-\infty}^{+\infty} J_P(t)\ dt) \ . \qquad (6)$$

The dynamics of $a(t)$ and $b(t)$ can be mapped to the evolution of a pseudospin in the presence of a time dependent effective magnetic field. The condition in Eq. (5a) means that the pseudospin makes a closed loop in the Bloch sphere, while the condition in Eq. (5b) ensures that the phase picked up by the pseudospin evolution during such a closed loop compensates the phase due to the potential exchange for a perfect $\sqrt{SWAP}$. The analytic solution for the evolution of a spin in a time dependent magnetic field can be found only in particular cases [9], and we will discuss here two of them: the Rabi solution [10], corresponding to a square pulse shape, and the Rosen and Zener solution [11] corresponding to a hyperbolic secant pulse shape.

The Rabi solution describes the precession of the pseudospin in a constant effective magnetic field. A square pulse in the tunnelling amplitude keeps this effective field on for a time T, and then turns it off. We can write the hopping term as a constant $\Omega(t) = \Omega$, and consider the time evolution given by the Rabi solution from a time $t = 0$ to $t = T$ (just the solution for t-independent H). In a similar way the potential exchange term $J_P(t) = J_P$ for $0 \le t \le T$ and zero otherwise. The probability of double occupancy at the end of the pulse is given by:

$$P_d(T) = |b(T)|^2 = \frac{\Omega^2/2}{\Omega^2 + \Delta^2}\sin^2\left(\frac{\sqrt{\Omega^2 + \Delta^2}}{2}T\right) \ . \qquad (7)$$

Therefore the condition in Eq. (5a) is satisfied by fixing the length of the pulse to

$$T_n = \frac{2n\pi}{\sqrt{\Omega^2 + \Delta^2}} \ . \qquad (8)$$

The integer n identifies the number of full precessions of the pseudospin during the pulse. We find from the Rabi solution that $a(T_n) = \exp(-i\Delta T_n/2)/\sqrt{2}$. Using this solution in Eq. (3), the condition in Eq. (5b) for the perfect $\sqrt{SWAP}$ is rewritten as

$$\cos n\pi\left(\frac{\Delta - 2J_P}{\sqrt{\Omega^2 + \Delta^2}}\right) = 0. \qquad (9)$$

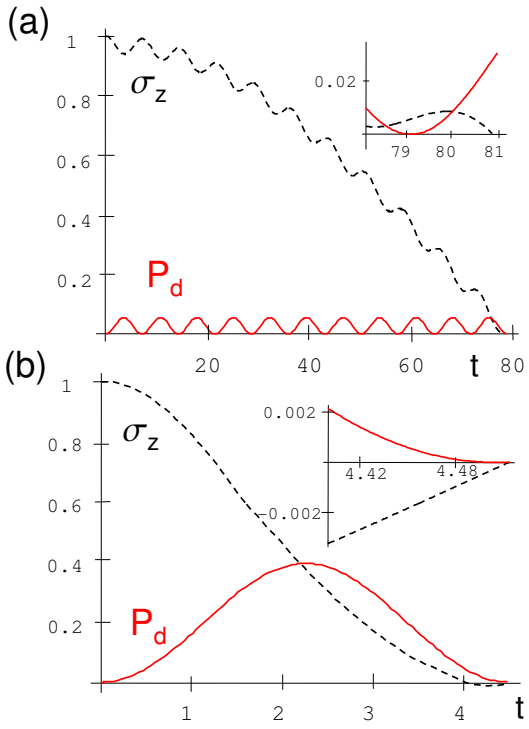

FIG. 1: $\sigma_z(t)$ and $P_d(t)$ for two electrons confined by hydrogenic potentials. Infinite tunnelling barriers are switched off during the time interval $0 < t < T$. Time t is in units of $\hbar/\mathrm{Ry}^*$. (a) The separation between the sites is 4.53 au*. At the end of the pulse we have a half swap with a small but nonzero P_d. (b) The separation is 2.38 au* and the energy levels satisfy the condition in Eq. (10). The half swap is realized in a shorter time and with $P_d = 0$ identically at the end of the pulse (see inset).

This can be recast in terms of the separation between the triplet and the lower singlet eigenvalues J, and the separation between the two *gerade* singlets ΔE as

$$\frac{2nJ}{\Delta E} = \frac{2k+1}{2}\ , \tag{10}$$

where k is any integer.

To illustrate the idea we show in Fig. 1 the evolution of $\sigma(t)$ and $P_d(t)$ in the square pulse case calculated assuming a hydrogenic confinement potential and localized functions of the Slater form, which models well the case of electrons confined in shallow donors. We want to stress that the general approach we are suggesting is independent of this particular choice. In fact, for any reasonable form of the confinement potential it is possible to modify the ratio in Eq. (10) by changing the maximum tunnelling amplitude or the separation between the dots/impurities. When the separation is large, so the overlap is small (or the tunnelling barrier is large), there is a small admixture of doubly-occupied states at any time. This is the region where the low-lying states are described accurately by the Heisenberg Hamiltonian $2J\mathbf{S}_a\cdot\mathbf{S}_b$. The spins here are associated with the sites; e.g. $S_a^+ = c_{a\uparrow}^\dagger c_{a\downarrow}$ [8]. This case is considered in Fig. 1 (a), obtained with a separation between the localized electrons of 4.53 au*. We indicate by au* and Ry* the atomic units scaled by the electron effective mass and the static dielectric constant. Time is in units of $\hbar/\mathrm{Ry}^*$. For a typical GaAs based system 1 Ry* $\sim$ 5 meV, 1 au* $\sim$ 80 Å, and $\hbar/Ry* \sim 0.1$ ps. We see that at the end of the pulse we satisfy the condition for the half swap $\sigma_z = 0$ with a small double occupancy $P_d \sim 0.03$ (see inset in Fig. 1 (a)). The new approach is illustrated in Fig. 1 (b) corresponding to a separation of 2.38 au*. At this separation the energy levels satisfy the condition in Eq. (10) yielding a perfect half swap with both $\sigma_z = 0$ and $P_d = 0$ identically. Fig. 1 (b) shows a marked increase in swap speed and a much higher probability of double occupancy during the gate compared to Fig. 1 (a). The case in Fig. 1 (b) corresponds to $n = 1$, higher n will give a perfect half swap in longer times.

The use of square pulses gives a direct illustration of the new approach. However, for practical purposes, a continuous time dependence of the pulse is desirable. Using the picture of the pseudospin in an effective magnetic field, we need to design in the general case a $\mathbf{B}_{eff}(t)$ that generates closed loops in the Bloch sphere. Once this first condition is realized, the condition on the control parameters for a perfect half swap can be found accordingly. This is possible for the hopping amplitude of the form $\Omega(t) = \Omega/\cosh(\pi t/T)$. Then $\int_{-\infty}^{+\infty}\Omega(t)\ dt = \Omega T$, the same as for the square pulse. The probability of double occupancy at the end of the pulse (at $t = +\infty$) can be obtained from the Rosen and Zener result [11]

$$P_d = \frac{\sin^2 \Omega T/2}{2\cosh^2 \Delta T/2}. \tag{11}$$

In the adiabatic approach the condition $\Delta T \gg 1$ in the denominator makes this probability small. Our approach takes advantage of the numerator in Eq. (11), which implies that for

$$T_n = \frac{2n\pi}{\Omega} \tag{12}$$

we will have no double occupancy at the end of the pulse. In order to determine the phase of $a(+\infty)$, we use the transformation $2z = \tanh(\pi t/T) + 1$ to map the infinite time interval to $[0, 1]$, and the equation for the coefficient $a(z)$ reads

$$(z^2 - z)a'' + \left(\frac{1}{2} + \frac{i\Delta T}{2\pi} - z\right)a' + \left(\frac{\Omega T}{2\pi}\right)^2 a = 0\ . \tag{13}$$

This is the hypergeometric equation and in general we obtain a solution in terms of a linear combination of hypergeometric functions. However, it is interesting to notice that if the condition for no double occupancy is met,

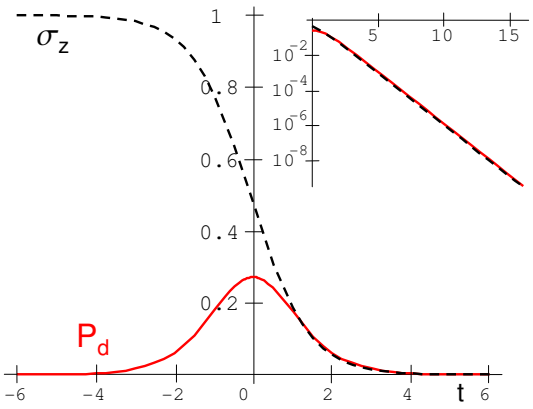

FIG. 2: $\sigma_z(t)$ and $P_d(t)$ for two electrons confined by hydrogenic potentials with barriers controlled using a hyperbolic secant pulse shape. The separation is $2.36\cdots$ au*. Time t is in units of $\hbar/\mathrm{Ry}^*$. The inset shows the Log of $\sigma(t)$ and $P_d(t)$ at longer times.

then $(\Omega T/2\pi) = n$, and we will fall in the degenerate case of the hypergeometric equation. As discussed in Ref. [12], the solution in this case consists of a polynomial of degree n. We find that the solution to Eq. (13) with the initial condition $a(0) = 1$ and with $|a(1)|^2 = 1$ can be written explicitly as $a_n(z) = n! P_n^{\alpha_n,\alpha_n^*}(1-2z)/(\alpha_n+1)_n$, where $P_n^{\beta,\gamma}(x)$ are Jacobi polynomials, $\alpha_n = -1/2 + in\Delta/\Omega$, and $(x)_n = \Gamma(x+n)/\Gamma(x)$. The condition in Eq. (5b) can then be written in a compact form using the hypergeometric function (which in this case terminates after n terms in the series) as

$$Re[F(-n, n, 1/2 + in\Delta/\Omega, 1)e^{i4nJ_P/\Omega}] = 0 \ , \qquad (14)$$

which is the parallel of Eq. (9) for this continuous pulse shape. The fact that the potential exchange $J_P(t)$ is $O(\Lambda^2)$ led us to take $J_P(t) = J_P \mathrm{sech}^2(t/T)$ in Eq. (14), although the solvability and essential aspects of the solution are not limited to this. We show in Fig. 2 the realization of a perfect half swap in the hydrogenic case. At the separation of about 2.36 au* the matrix elements of the Hamiltonian satisfy the condition in Eq. (14) and a perfect half swap can be realized. The case in Fig. 2 corresponds to $n = 1$ and we have checked that for higher n we can always find at least one separation to satisfy Eq. (14). The inset shows the exponential converging of P_d and σ_z toward the desired value. We remark that in GaAs based systems this translates in a half swap operated with an accuracy of 10^{-10} in a time of the order of 3 ps.

We now consider likely sources of error and other difficulties to be expected in a real implementation of the ideas proposed. We pose the question, if Ω and Δ deviate slightly from values needed for a perfect half-swap, how much do $\sigma(+\infty)$ and $P_d(+\infty)$ differ from their ideal values of zero? Using the analytic solutions we proved that if the deviation of the parameters is $O(\epsilon)$ then the deviation $\sigma(+\infty) = O(\epsilon)$ and $P_d(+\infty) = O(\epsilon^2)$. Higher intra-dot excitations will complicate our considerations. If they are large compared to $\hbar\Delta$, however, their effect will be small. To get an estimate of the requirements, consider these excitations for the infinite square well, side length L. Then $\delta E = 3\pi^2\hbar^2/2m^*L^2 = 6\pi^2(\mathrm{au}^*/L)^2\mathrm{Ry}^*$, is the first excitation energy, and $\hbar\Delta \approx 2e^2/(\epsilon L) = 2(\mathrm{au}^*/L)\mathrm{Ry}^*$, so $\delta E/\hbar\Delta \approx 3\pi^2(\mathrm{au}^*/L)$. For two GaAs quantum dots of lateral size $L = 100\mathring{A}$, this gives $\delta E/\hbar\Delta \approx 27$ and $\hbar\Delta \approx 2\mathrm{Ry}^*$, satisfying the requirement $\delta E/\hbar\Delta >> 1$. Finally, we remark that in order to take advantage of the proposed scheme the time resolution needed for controlling the gate is related to the intra-dot Coulomb repulsion $\hbar\Delta$. In principle, a subpicosecond switching time for a pulse gate is not out of the question [13]. By increasing the dot size L while maintaining a large $\delta E/\hbar\Delta$ it is possible to increase the resolution time Δ^{-1}. We estimate that this condition can be well satisfied for large ($\sim$ 300-400 Å) GaAs quantum dots in such a way to limit the resolution to the picosecond range, which is within state-of-the-art capabilities.

In conclusion, we have shown that by non-adiabatic control it is possible to take advantage of the double occupied states to make fast and accurate half swap operations. The idea can be applied to many systems currently under investigation for experimental realization of quantum computing. Even in systems where the mixing with double occupancy is small, the simple rules given here can be used as an error correction method. Possible generalizations to more than two spins [14] are under consideration. It is also of interest to consider more general pulse shapes, particularly with the object of seeing what forms of $\mathbf{B}_{eff}(t)$ will allow the pseudospin to return to its starting value (i.e. corresponding to $P_d = 0$).

We thank S. H. Tessmer, M. I. Dykman, and S. D. Mahanti for enlightening discussions. C.P. acknowledges support by NSF under contract DMR-0312491.

[1] M. Friesen, P. Rugheimer, D. E. Savage, M. G. Lagally, D. W. van der Weide, R. Joint, and M. A. Eriksson, Phys. Rev. B 76, 121301 (2003).
[2] D. Loss and D. P. DiVincenzo, Phys. Rev. A **57**, 120 (1998).
[3] R. Vrijen, E. Yablonovitch, K. Wang, H. W. Jiang, A. Balandin, V. Roychowdhury, T. Mor, and D. DiVincenzo, Phys. Rev. A **62**, 122306 (2000).
[4] X. Hu and S. Das Sarma, Phys. Rev. A **61**, 062301 (2000).
[5] J. Schliemann, D. Loss and A. H. MacDonald, Phys. Rev. B **63**, 085311 (2001).
[6] G. Burkard, D. Loss and D. P. DiVincenzo, Phys. Rev. B**59**, 2070 (1999).
[7] J. C. Slater, *Quantum Theory of Molecules and Solids* Vol.1, Chap.4 McGraw-Hill, New York (1963).

[8] P. W. Anderson, Solid State Physics **14**,99 (1963).
[9] A. M. Ishkhanyan, J. Phys. A **33**, 5539 (2000).
[10] L. Allen and J. H. Eberli, *Optical Resonance and Two-Level Atoms*, Wiley, New York 1975.
[11] N. Rosen and C. Zener, Phys. Rev. **40** 502 (1932).
[12] *Higher Trascendental Functions*, A. Erdélyi Editor, McGraw-Hill, New York (1953).
[13] S. Tessmer, private communication.
[14] D. A. Lidar and A. Mizel, cond-mat/0401081 (2004).